View metadata, citation and similar papers at core.ac.uk

brought to you by CORE

provided by Illinois Digital Environment for Access to Learning and Scholarship Repository

HIGH-RESOLUTION SPECTROSCOPY OF THE ν_{16} BAND OF 1,3,5-TRIOXANE

BRADLEY M. GIBSON, NICOLE KOEPPEN, *Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL, USA*; BENJAMIN J. McCALL, *Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL, USA*.

1,3,5-trioxane, often used as a solid fuel or source of formaldehyde, is a symmetric top of the C_{3v} group. Although the microwave[a] and low-resolution vibrational spectra[b] have been studied extensively, only the ν_{17} band near 1072 cm^{-1}has been observed with rotational resolution[c]. Here, we will present our studies of trioxane vapor from 1140-1220 cm^{-1}, covering the ν_{16} band at a resolution of approximately 30 MHz. Solid trioxane was heated, and the resulting vapor was entrained in a continuous supersonic expansion of argon. Continuous-wave cavity ringdown spectroscopy was then performed using a frequency-stabilized external cavity quantum cascade laser (EC-QCL) as the light source. In addition to providing new ro-vibrational transition frequencies of trioxane, the present work serves to validate our newly-developed EC-QCL spectrometer and will be used to evaluate the cooling performance of the sheath-flow supercritical fluid expansion source currently under development[d].

---

[a]Oka, T., Tsuchiya, K., Iwata, S., and Morino, Y. Microwave Spectrum of s-Trioxane. *Bull. Chem. Soc. Jpn.* **37** (1964), 4-7.

[b]Stair, A.T. Jr. and Nielsen, J. Rud. Vibrational Spectra of sym-Trioxane. *J. Chem. Phys.* **27** (1957), 402-407.

[c]Henninot, J-F., Bolvin, H., Demaison, J., and Lemoine, B. The Infrared Spectrum of Trioxane in a Supersonic Slit Jet. *J. Mol. Spect.* **152** (1992), 62-68.

[d]Gibson, B.M., Stewart, J.T., and McCall, B.J., contribution TJ14, presented at the 68th International Symposium on Molecular Spectroscopy, Columbus, OH, USA, 2013.